STN,
Inventor
search:
10·17·02

10/088425

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1610jxm

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | |
|---|---|---|
| NEWS 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS 2 | Apr 08 | "Ask CAS" for self-help around the clock |
| NEWS 3 | Apr 09 | BEILSTEIN: Reload and Implementation of a New Subject Area |
| NEWS 4 | Apr 09 | ZDB will be removed from STN |
| NEWS 5 | Apr 19 | US Patent Applications available in IFICDB, IFIPAT, and IFIUDB |
| NEWS 6 | Apr 22 | Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS |
| NEWS 7 | Apr 22 | BIOSIS Gene Names now available in TOXCENTER |
| NEWS 8 | Apr 22 | Federal Research in Progress (FEDRIP) now available |
| NEWS 9 | Jun 03 | New e-mail delivery for search results now available |
| NEWS 10 | Jun 10 | MEDLINE Reload |
| NEWS 11 | Jun 10 | PCTFULL has been reloaded |
| NEWS 12 | Jul 02 | FOREGE no longer contains STANDARDS file segment |
| NEWS 13 | Jul 22 | USAN to be reloaded July 28, 2002; saved answer sets no longer valid |
| NEWS 14 | Jul 29 | Enhanced polymer searching in REGISTRY |
| NEWS 15 | Jul 30 | NETFIRST to be removed from STN |
| NEWS 16 | Aug 08 | CANCERLIT reload |
| NEWS 17 | Aug 08 | PHARMAMarketLetter(PHARMAML) - new on STN |
| NEWS 18 | Aug 08 | NTIS has been reloaded and enhanced |
| NEWS 19 | Aug 19 | Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN |
| NEWS 20 | Aug 19 | IFIPAT, IFICDB, and IFIUDB have been reloaded |
| NEWS 21 | Aug 19 | The MEDLINE file segment of TOXCENTER has been reloaded |
| NEWS 22 | Aug 26 | Sequence searching in REGISTRY enhanced |
| NEWS 23 | Sep 03 | JAPIO has been reloaded and enhanced |
| NEWS 24 | Sep 16 | Experimental properties added to the REGISTRY file |
| NEWS 25 | Sep 16 | Indexing added to some pre-1967 records in CA/CAPLUS |
| NEWS 26 | Sep 16 | CA Section Thesaurus available in CAPLUS and CA |
| NEWS 27 | Oct 01 | CASREACT Enriched with Reactions from 1907 to 1985 |

| | |
|---|---|
| NEWS EXPRESS | October 14 CURRENT WINDOWS VERSION IS V6.01, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002 |
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS INTER | General Internet Information |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS PHONE | Direct Dial and Telecommunication Network Access to STN |
| NEWS WWW | CAS World Wide Web Site (general information) |

Enter NEWS followed by the item number or name to see news on that specific topic.

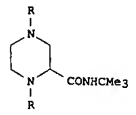
All use of STN is subject to the provisions of the STN Customer

```
=> E TAKASE MITSURU/AU 25
E1           67      TAKASE MITSUNORI/AU
E2           56      TAKASE MITSUO/AU
E3           19 --> TAKASE MITSURU/AU
E4            1      TAKASE MITUITIRO/AU
E5            2      TAKASE MITUNORI/AU
E6            4      TAKASE MITUO/AU
E7            1      TAKASE MIYUKI/AU
E8            1      TAKASE MORICHIKA/AU
E9            1      TAKASE MOTOHIRO/AU
E10           1      TAKASE MOTOYOSHI/AU
E11           1      TAKASE MUMEAKI/AU
E12          44      TAKASE MUNEAKI/AU
E13           8      TAKASE N/AU
E14           4      TAKASE NAGATAKE/AU
E15           8      TAKASE NAME NOT TRANSLATED/AU
E16           3      TAKASE NAOAKI/AU
E17           5      TAKASE NAOKI/AU
E18           5      TAKASE NAOKO/AU
E19           1      TAKASE NAOSHI/AU
E20           1      TAKASE NATSUKO/AU
E21           9      TAKASE NOBORU/AU
E22           1      TAKASE NOBUAKI/AU
E23          37      TAKASE NOBUMITSU/AU
E24           9      TAKASE NOBUO/AU
E25           1      TAKASE NOBUTAKE/AU

=> S (E3) AND (CARBOXAMID?)
            19 "TAKASE MITSURU"/AU
         16882 CARBOXAMID?
L15           2 ("TAKASE MITSURU"/AU) AND (CARBOXAMID?)

=> s l15 not l9
L16           1 L15 NOT L9

=> d l16 ibib abs hitstr
```

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:120860 CAPLUS
DOCUMENT NUMBER: 132:180586
TITLE: Method for preparation of piperazine-2-**carboxamide** derivatives
INVENTOR(S): Hirai, Yukio; **Takase, Mitsuru**; Takata, Mitsumasa; Nagasaki, Fumihiko
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 2000053656 | A2 | 20000222 | JP 1998-238001 | 19980810 |

OTHER SOURCE(S): CASREACT 132:180586; MARPAT 132:180586
GI




I

AB The title compds. [I; R = H, Bn (benzyl)] are prepd. by cyclocondensation of N-tert-butyl-3-halo-2-hydroxypropanamide [XCH2CH(OH)CONHCMe3] with N,N'-dibenzylethylenediamine (BnNHCH2CH2NHBn). This process neither uses expensive platinum oxide nor specialized app. and gives N-tert-butyl-2-piperazinecarboxamide in good yields in an industrially advantageous manner, which is useful as an intermediate for drugs or agrochems. Thus, epoxidn. of N-tert-butylacrylamide with m-chloroperbenzoic acid in CHCl3 at room temp. for 100 h gave 58.0% N-tert-butyl-2,3-epoxypropanamide which was dissolved in CHCl3 and treated with concd. HCl at room temp. for 30 min to quant. give N-tert-butyl-3-chloro-2-hydroxypropanamide. Mesylation of the latter compd. with methanesulfonyl chloride in the presence of Et3N at room temp. for 1 h gave 72.6% N-tert-butyl-3-chloro-2-(methanesulfonyloxy)propanamide which underwent cyclocondensation with N,N'-dibenzylethylenediamine in the

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS (Continued)
presence of DBU under reflux for 5 h to give 83.2% N-tert-butyl-1,4-dibenzyl-2-piperazinecarboxamide, I (R = Bn) and 10.5% CH2:CH(OSO2Me)CONHCMe3.

```
=> E YAMAZAKI SATORU/AU 25
E1            3     YAMAZAKI SATOKO/AU
E2            2     YAMAZAKI SATOMI/AU
E3           81 --> YAMAZAKI SATORU/AU
E4          173     YAMAZAKI SATOSHI/AU
E5            2     YAMAZAKI SATOYUKI/AU
E6            2     YAMAZAKI SAYAKA/AU
E7            8     YAMAZAKI SAYURI/AU
E8            1     YAMAZAKI SCIICHIRO/AU
E9            8     YAMAZAKI SEI/AU
E10           1     YAMAZAKI SEI ICHIRO/AU
E11           2     YAMAZAKI SEIETSU/AU
E12           6     YAMAZAKI SEIHACHIRO/AU
E13          30     YAMAZAKI SEIICHI/AU
E14          60     YAMAZAKI SEIICHIRO/AU
E15           1     YAMAZAKI SEIICHIROU/AU
E16         122     YAMAZAKI SEIJI/AU
E17           3     YAMAZAKI SEIJIRO/AU
E18           1     YAMAZAKI SEIJU/AU
E19           1     YAMAZAKI SEIKI/AU
E20           8     YAMAZAKI SEIRO/AU
E21           1     YAMAZAKI SEISAKU/AU
E22           2     YAMAZAKI SEISHI/AU
E23           1     YAMAZAKI SEIZI/AU
E24           1     YAMAZAKI SENE/AU
E25           1     YAMAZAKI SENJI/AU

=> S (E3) AND (CARBOXAMID?)
            81 "YAMAZAKI SATORU"/AU
         16882 CARBOXAMID?
L17          2 ("YAMAZAKI SATORU"/AU) AND (CARBOXAMID?)

=> s l17 not l9
L18          1 L17 NOT L9

=> s l18 not l10
L19          1 L18 NOT L10

=> s l19 not l12
L20          1 L19 NOT L12

=> d l20 ibib abs hitstr
```

L20 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:420276 CAPLUS
DOCUMENT NUMBER: 127:130827
TITLE: KMD-3213, a novel .alpha.1A-adrenoceptor antagonist, potently inhibits the functional .alpha.1-adrenoceptor in human prostate
AUTHOR(S): Moriyama, Nobuo; Akiyama, Katsuyoshi; Murata, Satoshi; Taniguchi, Jun; Ishida, Norio; Yamazaki, Satoru; Kawabe, Kazuki
CORPORATE SOURCE: Department of Urology, Faculty of Medicine, The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo, 113, Japan
SOURCE: European Journal of Pharmacology (1997), 331(1), 39-42
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB KMD-3213, (-)-(R)-1-(3-hydroxypropyl)-5-[2-[[2-[2-(2,2,2-trifluoroethoxy)phenoxy]ethyl]amino]propyl]indoline-7-carboxamide, is a novel and selective .alpha.1A-adrenoceptor antagonist. The potency of this drug to antagonize functional .alpha.1-adrenoceptor-mediated contraction in human prostatic smooth muscle was evaluated and compared with that of other .alpha.1-adrenoceptor antagonists. KMD-3213 inhibited noradrenaline-induced contractions with an apparent pKB value of 9.45, indicating a potency similar to that of tamsulosin. The affinity of prazosin for prostatic .alpha.1-adrenoceptors is given as potency for the .alpha.1L-adrenoceptor with an estd. pA2 value of 8.84. The data obtained in this study suggest that KMD-3213, an .alpha.1A-adrenoceptor-selective antagonist, has strong affinity for the .alpha.1L-adrenoceptor in the human prostate.

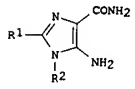
```
=> E ISHII YUTAKA/AU 25
E1            7      ISHII YUSUKE/AU
E2            1      ISHII YUSUNOBU/AU
E3           87 --> ISHII YUTAKA/AU
E4            1      ISHII YUTARO/AU
E5            1      ISHII YUTOKU/AU
E6            4      ISHII YUU/AU
E7            3      ISHII YUUJI/AU
E8            1      ISHII YUUKI/AU
E9           22      ISHII YUUKO/AU
E10          11      ISHII YUZO/AU
E11           1      ISHII YUZOU/AU
E12           1      ISHII ZENICHI/AU
E13          12      ISHII ZENSHO/AU
E14           1      ISHIIA C/AU
E15           1      ISHIIB M/AU
E16           2      ISHIIDA CHIAKI/AU
E17           1      ISHIIDA H/AU
E18           1      ISHIIDA KAZUAKI/AU
E19           1      ISHIIDA RYOJI/AU
E20           1      ISHIIDE AKITOSHI/AU
E21           3      ISHIIDE HIDEKI/AU
E22           8      ISHIIDE TAKASHI/AU
E23           4      ISHIIE SHUNJI/AU
E24           8      ISHIIE TATSUJI/AU
E25           1      ISHIIGAME M/AU

=> S (E3) AND (CARBOXAMID?)
             87 "ISHII YUTAKA"/AU
          16882 CARBOXAMID?
L21           1 ("ISHII YUTAKA"/AU) AND (CARBOXAMID?)

=> d l21 ibib abs hitstr
```

L21 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:228862 CAPLUS
DOCUMENT NUMBER: 134:252338
TITLE: Processes for the preparation of 4(5)-amino-5(4)-**carboxamidoimidazoles** and intermediates thereof
INVENTOR(S): Shibasaki, Hiroaki; Nagasaki, Fumihiko; Takase, Mitsuru; Yamazaki, Satoru; **Ishii, Yutaka**; Oohata, Kimihiko
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan; Ibaraki Kasei Co., Ltd.
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001021592 | A1 | 20010329 | WO 2000-JP6397 | 20000920 |
| W: CN, IN, KR, US | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| JP 2001151760 | A2 | 20010605 | JP 1999-330103 | 19991119 |
| JP 2001302609 | A2 | 20011031 | JP 2000-116218 | 20000418 |
| JP 2001158776 | A2 | 20010612 | JP 2000-284780 | 20000920 |
| EP 1215206 | A1 | 20020619 | EP 2000-961096 | 20000920 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY | | | | |

PRIORITY APPLN. INFO.:
JP 1999-264818 A 19990920
JP 1999-330103 A 19991119
JP 2000-116218 A 20000418
WO 2000-JP6397 W 20000920

OTHER SOURCE(S): CASREACT 134:252338; MARPAT 134:252338
GI



I

AB The invention provides novel processes for prepg. efficiently compds. of general formula (I) (wherein R1 and R2 are each independently hydrogen, optionally substituted C1-10 alkyl, C3-14 hydrocarbyl bearing an alicyclic skeleton, optionally substituted alkynyl, optionally substituted aryl,

L21 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS (Continued)
optionally substituted aralkyl, optionally substituted heterocyclyl, optionally substituted heterocyclylalkyl, N-optionally substituted carbamoyl, or alkoxycarbonyl) and intermediates thereof. Compds. of general formula I can be prepd. by subjecting compds. of general formula R2NHC(R1):NC(CN):C(NH2)CN (II; R1 and R2 are defined above) and/or salts thereof to cyclization hydrolysis in an aq. basic soln. Further, compds. of general formula II can be prepd. from industrially easily available diaminomaleonitrile in a high yield. The compds. I are useful as intermediates for agrochems. and drugs, e.g. dacarbazine and temozoromide (anticancer agent) and urazamide (liver-protective agent). Thus, 50 mL H2O and 43.0 g 25% NaOH were added to 8.0 g N-(2-amino-1,2-dicyanovinyl)formamidine and refluxed for 2 h, cooled to room temp., neutralized with 35% HCl to pH 7, concd. to dryness, treated with ethanol, and filtered for removing the insol. salt. The filtrate was treated with activated charcoal, filtered, and concd. to give a soln. of 4(5)-aminoimidazole-5-**carboxamide** (III) which was adjusted to pH .ltoreq.3 and cooled at .ltoreq.10.degree.. The pptd. crystals were collected by filtration and dried to give 84% III.HCl.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
=> E OOHATA KIMIHIKO/AU 25
E1            2     OOHATA KENICHI/AU
E2            2     OOHATA KENJI/AU
E3            1 --> OOHATA KIMIHIKO/AU
E4            2     OOHATA KIMIO/AU
E5            8     OOHATA KIMITAKA/AU
E6            5     OOHATA KIYOSHI/AU
E7            6     OOHATA KIYOSI/AU
E8            1     OOHATA KOHEI/AU
E9            3     OOHATA KOICHI/AU
E10           2     OOHATA KOJI/AU
E11           1     OOHATA KOKI/AU
E12           2     OOHATA KOKICHI/AU
E13           1     OOHATA KOUBUN/AU
E14           1     OOHATA KUNIHIRO/AU
E15           1     OOHATA KUSHIRO/AU
E16           1     OOHATA KYOUSHI/AU
E17          10     OOHATA MANABU/AU
E18           1     OOHATA MASAHIRO/AU
E19           2     OOHATA MASASHI/AU
E20           5     OOHATA MASATO/AU
E21           3     OOHATA MASATOSHI/AU
E22           1     OOHATA MITSUGU/AU
E23           2     OOHATA MITSURU/AU
E24           1     OOHATA NAME NOT TRANSLATED/AU
E25           6     OOHATA NOBUTAKA/AU

=> S (E3 OR E4) AND (CARBOXAMID?)
              1 "OOHATA KIMIHIKO"/AU
              2 "OOHATA KIMIO"/AU
          16882 CARBOXAMID?
L22           1 ("OOHATA KIMIHIKO"/AU OR "OOHATA KIMIO"/AU) AND (CARBOXAMID?)

=> s l22 not l9
L23           0 L22 NOT L9

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                   52.69     342.22

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -5.58      -5.58

STN INTERNATIONAL LOGOFF AT 08:13:18 ON 17 OCT 2002
```

Connecting via Winsock to STN

Welcome to STN International! Enter x:X

LOGINID:ssspta1626amd

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | |
|---|---|---|
| NEWS 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS 2 | Apr 08 | "Ask CAS" for self-help around the clock |
| NEWS 3 | Apr 09 | BEILSTEIN: Reload and Implementation of a New Subject Area |
| NEWS 4 | Apr 09 | ZDB will be removed from STN |
| NEWS 5 | Apr 19 | US Patent Applications available in IFICDB, IFIPAT, and IFIUDB |
| NEWS 6 | Apr 22 | Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS |
| NEWS 7 | Apr 22 | BIOSIS Gene Names now available in TOXCENTER |
| NEWS 8 | Apr 22 | Federal Research in Progress (FEDRIP) now available |
| NEWS 9 | Jun 03 | New e-mail delivery for search results now available |
| NEWS 10 | Jun 10 | MEDLINE Reload |
| NEWS 11 | Jun 10 | PCTFULL has been reloaded |
| NEWS 12 | Jul 02 | FOREGE no longer contains STANDARDS file segment |
| NEWS 13 | Jul 22 | USAN to be reloaded July 28, 2002; saved answer sets no longer valid |
| NEWS 14 | Jul 29 | Enhanced polymer searching in REGISTRY |
| NEWS 15 | Jul 30 | NETFIRST to be removed from STN |
| NEWS 16 | Aug 08 | CANCERLIT reload |
| NEWS 17 | Aug 08 | PHARMAMarketLetter(PHARMAML) - new on STN |
| NEWS 18 | Aug 08 | NTIS has been reloaded and enhanced |
| NEWS 19 | Aug 19 | Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN |
| NEWS 20 | Aug 19 | IFIPAT, IFICDB, and IFIUDB have been reloaded |
| NEWS 21 | Aug 19 | The MEDLINE file segment of TOXCENTER has been reloaded |
| NEWS 22 | Aug 26 | Sequence searching in REGISTRY enhanced |
| NEWS 23 | Sep 03 | JAPIO has been reloaded and enhanced |
| NEWS 24 | Sep 16 | Experimental properties added to the REGISTRY file |
| NEWS 25 | Sep 16 | Indexing added to some pre-1967 records in CA/CAPLUS |
| NEWS 26 | Sep 16 | CA Section Thesaurus available in CAPLUS and CA |
| NEWS 27 | Oct 01 | CASREACT Enriched with Reactions from 1907 to 1985 |

| | |
|---|---|
| NEWS EXPRESS | October 14 CURRENT WINDOWS VERSION IS V6.01, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002 |
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS INTER | General Internet Information |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS PHONE | Direct Dial and Telecommunication Network Access to STN |
| NEWS WWW | CAS World Wide Web Site (general information) |

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:57:19 ON 16 OCT 2002

=> fil reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 15:57:26 ON 16 OCT 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 OCT 2002 HIGHEST RN 461638-40-4
DICTIONARY FILE UPDATES: 15 OCT 2002 HIGHEST RN 461638-40-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10088425.str

L1 STRUCTURE UPLOADED

=> s l1 ful
FULL SEARCH INITIATED 15:57:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2532 TO ITERATE

100.0% PROCESSED 2532 ITERATIONS 560 ANSWERS
SEARCH TIME: 00.00.01

L2 560 SEA SSS FUL L1

=>
Uploading 100884251.str

L3 STRUCTURE UPLOADED

```
=> s l3 ful
FULL SEARCH INITIATED 15:59:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    209 TO ITERATE

100.0% PROCESSED     209 ITERATIONS                          89 ANSWERS
SEARCH TIME: 00.00.01

L4           89 SEA SSS FUL L3

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             281.32     281.53

FILE 'CAPLUS' ENTERED AT 15:59:33 ON 16 OCT 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 16 Oct 2002  VOL 137 ISS 16
FILE LAST UPDATED: 15 Oct 2002  (20021015/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

CAS roles have been modified effective December 16, 2001. Please
check your SDI profiles to see if they need to be revised. For
information on CAS roles, enter HELP ROLES at an arrow prompt or use
the CAS Roles thesaurus (/RL field) in this file.

=> s l2/p
L5          302 L2/P

=> d his

     (FILE 'HOME' ENTERED AT 15:57:19 ON 16 OCT 2002)

     FILE 'REGISTRY' ENTERED AT 15:57:26 ON 16 OCT 2002
L1              STRUCTURE UPLOADED
L2           560 S L1 FUL
L3              STRUCTURE UPLOADED
L4            89 S L3 FUL

     FILE 'CAPLUS' ENTERED AT 15:59:33 ON 16 OCT 2002
L5           302 S L2/P

=> s l5 and l4
```

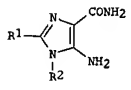
```
             35 L4
L6            4 L5 AND L4

=> d 1-4 ibib abs hitstr
```

L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:228862 CAPLUS
DOCUMENT NUMBER: 134:252338
TITLE: Processes for the preparation of 4(5)-amino-5(4)-carboxamidoimidazoles and intermediates thereof
INVENTOR(S): Shibasaki, Hiroaki; Nagasaki, Fumihiko; Takase, Mitsuru; Yamazaki, Satoru; Ishii, Yutaka; Oohata, Kimihiko
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan; Ibaraki Kasei Co., Ltd.
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001021592 | A1 | 20010329 | WO 2000-JP6397 | 20000920 |
| W: CN, IN, KR, US | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| JP 2001151760 | A2 | 20010605 | JP 1999-330103 | 19991119 |
| JP 2001302609 | A2 | 20011031 | JP 2000-116218 | 20000418 |
| JP 2001158776 | A2 | 20010612 | JP 2000-284780 | 20000920 |
| EP 1215206 | A1 | 20020619 | EP 2000-961096 | 20000920 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY | | | | |

PRIORITY APPLN. INFO.: JP 1999-264818 A 19990920
JP 1999-330103 A 19991119
JP 2000-116218 A 20000418
WO 2000-JP6397 W 20000920

OTHER SOURCE(S): CASREACT 134:252338; MARPAT 134:252338
GI

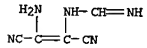


I

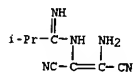
AB The invention provides novel processes for prepg. efficiently compds. of general formula (I) (wherein R1 and R2 are each independently hydrogen, optionally substituted C1-10 alkyl, C3-14 hydrocarbyl bearing an alicyclic skeleton, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, optionally substituted heterocyclyl, optionally substituted heterocyclylalkyl, N-optionally substituted carbamoyl, or alkoxycarbonyl) and intermediates thereof. Compds. of general formula I can be prepd. by subjecting compds. of general formula R2NHC(R1):NC(CN):C(NH2)CN (II; R1 and R2 are defined above) and/or salts thereof to cyclization hydrolysis in an aq. basic soln. Further, compds. of general formula II can be prepd. from industrially easily available diaminomaleonitrile in a high yield. The compds. I are useful as intermediates for agrochems. and drugs, e.g. dacarbazine and temozoromide (anticancer agent) and urazamide (liver-protective agent). Thus, 50 mL H2O and 43.0 g 25% NaOH were added to 8.0 g N-(2-amino-1,2-dicyanovinyl)formamidine and refluxed for 2 h, cooled to room temp., neutralized with 35% HCl to pH 7, concd. to dryness, treated with ethanol, and filtered for removing the insol. salt. The filtrate was treated with activated charcoal, filtered, and concd. to give a soln. of 4(5)-aminoimidazole-5-carboxamide (III) which was adjusted to pH .ltoreq.3 and cooled at .ltoreq.10.degree.. The pptd. crystals were collected by filtration and dried to give 84% III.HCl.

IT **331282-40-7P**, N-(2-Amino-1,2-dicyanovinyl)formamidine
**331282-41-8P**, N-(2-Amino-1,2-dicyanovinyl)isobutyramidine hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of aminocarboxamidoimidazoles as intermediates for anticancer and liver-protective agents by cyclization of (aminodicyanovinyl)formamidine derivs.)

RN 331282-40-7 CAPLUS
CN Methanimidamide, N-(2-amino-1,2-dicyanoethenyl)- (9CI) (CA INDEX NAME)



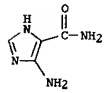
RN 331282-41-8 CAPLUS
CN Propanimidamide, N-(2-amino-1,2-dicyanoethenyl)-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

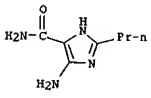
IT **72-40-2P**, 4-Aminoimidazole-5-carboxamide hydrochloride
**90521-73-6P**, 5-Amino-2-propyl-1H-imidazole-4-carboxamide
**227078-19-5P**, 5-Amino-2-isopropyl-1H-imidazole-4-carboxamide
**331282-42-9P**, N-(2-Amino-1,2-dicyanovinyl)butyramidine hydrochloride
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of aminocarboxamidoimidazoles as intermediates for anticancer and liver-protective agents by cyclization of (aminodicyanovinyl)formamidine derivs.)

RN 72-40-2 CAPLUS
CN 1H-Imidazole-4-carboxamide, 5-amino-, monohydrochloride (9CI) (CA INDEX NAME)

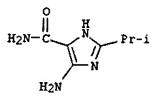


● HCl

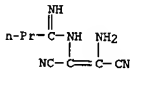
RN 90521-73-6 CAPLUS
CN 1H-Imidazole-4-carboxamide, 5-amino-2-propyl- (9CI) (CA INDEX NAME)



RN 227078-19-5 CAPLUS
CN 1H-Imidazole-4-carboxamide, 5-amino-2-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 331282-42-9 CAPLUS
CN Butanimidamide, N-(2-amino-1,2-dicyanoethenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

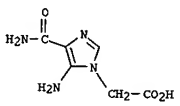
L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:270332 CAPLUS
DOCUMENT NUMBER: 133:85826
TITLE: Peptide nucleic acids rather than RNA may have been the first genetic molecule
AUTHOR(S): Nelson, Kevin E.; Levy, Matthew; Miller, Stanley L.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0506, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2000), 97(8), 3868-3871
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Numerous problems exist with the current thinking of RNA as the first genetic material. No plausible prebiotic processes have yet been demonstrated to produce the nucleosides or nucleotides or for efficient two-way nonenzymic replication. Peptide nucleic acid (PNA) is a promising precursor to RNA, consisting of N-(2-aminoethyl)glycine (AEG) and the adenine, uracil, guanine, and cytosine-N-acetic acids. However, PNA has not yet been demonstrated to be prebiotic. We show here that AEG is produced directly in elec. discharge reactions from CH4, N2, NH3, and H2O. Elec. discharges also produce ethylenediamine, as do NH4CN polymns. AEG is produced from the robust Strecker synthesis with ethylenediamine. The NH4CN polymn. in the presence of glycine leads to the adenine and guanine-N9-acetic acids, and the cytosine and uracil-N1-acetic acids are produced in high yield from the reaction of cyanoacetaldehyde with hydantoic acid, rather than urea. Preliminary expts. suggest that AEG may polymerize rapidly at 100.degree. to give the polypeptide backbone of PNA. The ease of synthesis of the components of PNA and possibility of polymn. of AEG reinforce the possibility that PNA may have been the first genetic material.

IT **112630-45-2P 281676-74-2P**
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(role of PNA in prebiotic mol. evolution)

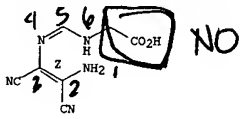
RN 112630-45-2 CAPLUS

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2002 ACS (Continued)
CN 1H-Imidazole-1-acetic acid, 5-amino-4-(aminocarbonyl)- (9CI) (CA INDEX NAME)



RN 281676-74-2 CAPLUS
CN Glycine, N-{[[(1Z)-2-amino-1,2-dicyanoethenyl]amino]methylene}- (9CI) (CA INDEX NAME)

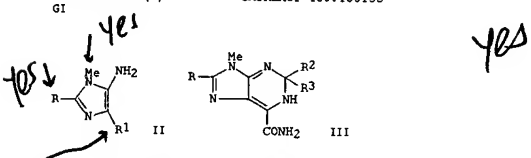
Double bond geometry as shown.



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

submitted in IDS

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:150133 CAPLUS
DOCUMENT NUMBER: 108:150133
TITLE: Chemistry of nitrilium salts. Part 4. Some reactions of 5-amino-4-(C-cyanoformimidoyl)imidazoles obtained from nitrilium trifluoromethanesulfonate salts and diaminomaleonitrile
AUTHOR(S): Booth, Brian L.; Coster, Ronald D.; Fernanda, M.; Proenca, J. R. P.
CORPORATE SOURCE: Inst. Sci. Technol., Univ. Manchester, Manchester, M60 1QD, UK
SOURCE: J. Chem. Soc., Perkin Trans. 1 (1987), (7), 1521-6
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:150133
GI



II III

AB Diaminomaleonitrile reacted readily with RC.tplbond.N+Me O3-SCF3 (R = Me, Ph) to give MeNHC+RNHC(CN):C(CN)NH2 O3-SCF3 (I; R = Me, Ph), which on base treatment under different conditions gave imidazoles II [R1 = cyano, CONH2, C(CN):NH]. I reacted with aldehydes and ketones at room temp. to give trifluorometanesulfonate salts of dihydropurines III [R = Me, Ph; R2 = Me, H; R3 = Me, Ph; R2R3 = (CH2)4]. Similarly II [R = Me, R1 = C(CN):NH] reacted with aldehydes, ketones, 1,2- and 1,3-diketones and keto esters to give dihydropurines III (R = R2 = Me, R3 = Me, Et, Ph, COMe, CH2CO2Et, CO2Et, CH2COMe; R = Me, R2 = Ph, R3 = H, Bz) some of which oxidized in air to purines.

IT **112995-31-0P 112995-33-2P 112995-35-4P 113684-62-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of, with aldehydes and ketones, purines from)

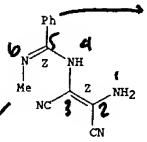
RN 112995-31-0 CAPLUS
CN Methanesulfonic acid, trifluoro-, compd. with (Z,Z)-N-(2-amino-1,2-dicyanoethenyl)-N'-methylbenzenecarboximidamide (1:1) (9CI) (CA INDEX NAME)

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS (Continued)

CM 1

CRN 112995-30-9
CMF C12 H11 N5

Double bond geometry as shown.



$R_1$ = aryl group ⟩ yes.

$R_2$ = alkyl

CM 2

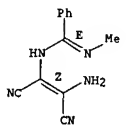
CRN 1493-13-6
CMF C H F3 O3 S

RN 112995-33-2 CAPLUS
CN Methanesulfonic acid, trifluoro-, compd. with (Z,E)-N-(2-amino-1,2-dicyanoethenyl)-N'-methylbenzenecarboximidamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112995-32-1
CMF C12 H11 N5

Double bond geometry as shown.



L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS (Continued)

CM 2

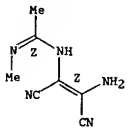
CRN 1493-13-6
CMF C H F3 O3 S

RN 112995-35-4 CAPLUS
CN Methanesulfonic acid, trifluoro-, compd. with (Z,Z)-N-(2-amino-1,2-dicyanoethenyl)-N'-methylethanimidamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112995-34-3
CMF C7 H9 N5

Double bond geometry as shown.



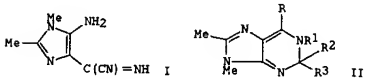
CM 2

CRN 1493-13-6
CMF C H F3 O3 S

RN 113684-62-1 CAPLUS
CN Methanesulfonic acid, trifluoro-, compd. with (Z,E)-N-(2-amino-1,2-dicyanoethenyl)-N'-methylethanimidamide (1:1) (9CI) (CA INDEX NAME)

CM 1

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:19863 CAPLUS
DOCUMENT NUMBER: 96:19863
TITLE: Synthesis of 6-cyano- and 6-carbamoylpurines and 6-carbamoyl-1,2-dihydropurines from N-methylacetonitrilium trifluoromethanesulfonate and diaminomaleonitrile
AUTHOR(S): Booth, Brian L.; Proenca, M. Fernanda
CORPORATE SOURCE: Dep. Chem., Univ. Manchester Inst. Sci. Technol., Manchester, M60 1QD, UK
SOURCE: J. Chem. Soc., Chem. Commun. (1981), (15), 788-9
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB NCC(NH2):C(NH2)CN reacted with [MeC.tplbond.NMe]+ -O3SCF3 to give, after controlled basification (pH 8-9, Na2CO3), 80% imidazole I, which forms 6-cyanopurines with carboxylic acid anhydrides, and with aldehydes, ketones, 1,2- and 1,3-diketones, and keto esters gives 6-carbamoyl-1,2-dihydropurine derivs. from which 6-carbamoylpurines can be obtained. Thus, I with Ac2O gave 80% purine II (R = CN, R1R2 = bond, R3 = Me), whereas I with MeCOCH2CO2Et gave 80% II (R = CONH2, R1 = H, R2 = CH2CO2Et, R3 = Me) which on standing in CHCl3 or EtOH (20.degree., 1-2 days) gave 73% II (R = CONH2, R1R2 = bond, R3 = Me).

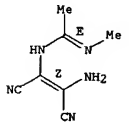
IT **80052-78-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of)
RN 80052-78-4 CAPLUS
CN Ethanimidamide, N-(2-amino-1,2-dicyanoethenyl)-N'-methyl-, conjugate monoacid, (Z,?)- (9CI) (CA INDEX NAME)

Double bond geometry as described by E or Z.

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS (Continued)

CRN 113684-61-0
CMF C7 H9 N5

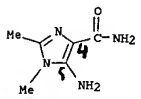
Double bond geometry as shown.



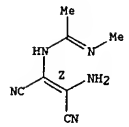
CM 2

CRN 1493-13-6
CMF C H F3 O3 S

IT **78750-93-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 78750-93-3 CAPLUS
CN 1H-Imidazole-4-carboxamide, 5-amino-1,2-dimethyl- (9CI) (CA INDEX NAME)

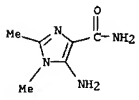


L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2002 ACS (Continued)



● H+

IT **78750-93-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 78750-93-3 CAPLUS
CN 1H-Imidazole-4-carboxamide, 5-amino-1,2-dimethyl- (9CI) (CA INDEX NAME)



=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 17.95 | 299.48 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -2.48 | -2.48 |

STN INTERNATIONAL LOGOFF AT 16:00:17 ON 16 OCT 2002